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Anomalous diffusion in quasi-one-dimensional systems

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Abstract

In order to perform quantum Hamiltonian dynamics minimizing localization effects, we introduce a quasi-one-dimensional tight-binding model whose mean free path is smaller than the size of the sample. This size, in turn, is smaller than the localization length. We study the return probability to the starting layer using direct diagonalization of the Hamiltonian. We create a one-dimensional excitation and observe sub-diffusive behavior for times larger than the Debye time but shorter than the Heisenberg time. The exponent corresponds to the fractal dimension $d^* \sim 0.72$ which is compared to that calculated from the eigenstates by means of the inverse participation number.

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The classical kinetic theory predicts that, in a disordered system, the return probability of an excitation decays with a diffusive law $P(t) \sim (4\pi Dt)^{-d/2}$, where D is the diffusion coefficient and d the dimension of the system. This fact has been extensively used in many areas of physics, in particular in electronic transport. However, the theory of quantum localization [1], on the basis of steady state transport properties, made clear that different regimes arise as a function of the disorder W. For $W \to \infty$, the eigenstates are completely localized and wave packets do not move through the system (insulating phase). If $W \to 0$, the motion is completely ballistic with a velocity $Ja/\hbar$. Between these two limits the diffusive behavior (metallic phase) is observed. The particles move around freely between collisions for a certain average length ℓ, called the mean free path.

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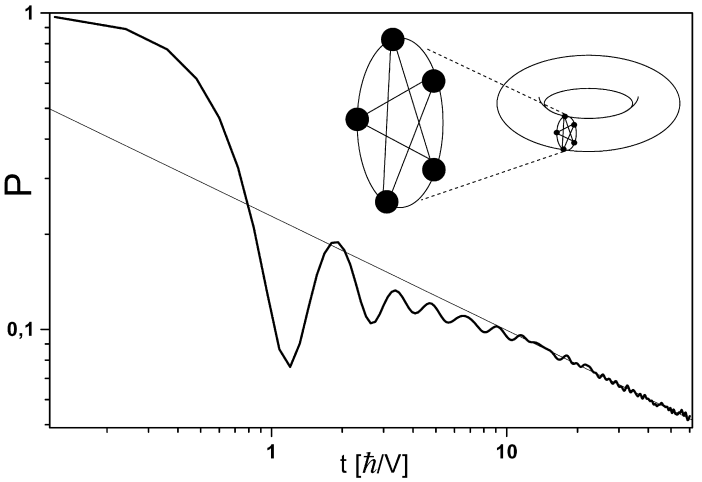

Fig. 1. Evolution of the layer autocorrelation function (in thick solid line). The thin line is a best fit to $(4\pi Dt)^{d^*/2}$, with the results $d^* = 0.72 \pm 0.005$ and $D = (4.84 \pm 0.08)a^2V/\hbar$. In the inset a schematics of the system is shown. As shown in the inset, the layers are fully connected, and periodic boundary conditions are applied to the longitudinal dimension.

More recently, theoretical studies have considered the regime where the critical amount of disorder W_C is such that the system is at the metal–insulator transition ($W_C \sim zJ$ is the typical exchange energies with z neighbors at distance a). In that case, the dynamics of the system is diffusive, but with a smaller exponent implying $d^* < d$ [2]. This reduction in the effective dimension is attributed to the (multi) fractality of the eigenstates at the transition. On the other hand, the diffusion of a spin excitation was directly observed [3] in NMR experiments. When the spin network has a cubic structure filling the space, the intensity of the excitation decays as $(t - t_0)^{-1.5}$, which is the expected value for diffusion in a three-dimensional system. However, the same experiment performed in a chain-like structure (powdered polyethylene) shows anomalous exponents in the diffusion of the excitation; namely 0.9 and 0.7 for the crystalline and amorphous parts of the sample, respectively. In these systems, the role of disorder is played by typical energy differences W between states, which are smaller than exchange energies zJ. This assures [4] a diffusive dynamics with [5] $D \sim Ja^2/\hbar$. Therefore, the effective dimensions $d^* = 1.8$ and 1.4 corresponding to these values reflect the spatial structure of the spin network.

In this work we study the conditions to reach the diffusive regime from actual quantum dynamics, namely the numerical study of model Hamiltonians. In particular, we developed a quasi-one-dimensional tight binding model system, which we called *the Stars necklace model*, whose basic unit (layer) is a highly connected cluster (see the inset of Fig. 1) with N sites and intralayer hopping $T = V/\sqrt{N}$. Disorder is introduced through on-site energies characterized by a random distribution of width W. The initial wave function is a packet defined in one layer of the system. We are interested in the probability of return to the layer, P, which is the sum of probabilities of finding the particle

in every site of the initial layer. To calculate the dynamics of the system we perform an exact diagonalization of the Hamiltonian. One key aspect of the numerical calculation is that the mean free path ℓ, the size of the system L and the localization length ξ must obey some restrictive relationships. The condition for a diffusive regime is ℓ much smaller than L, hence assuring that the particle will collide many times before reaching the boundaries of the system. In turn, to stay away from the localized regime, L must be smaller than ξ. For a strictly one-dimensional wire $\xi = 2\ell$, while for strips and bars with a given number of transverse modes (channels) M the localization length is expected to go [6] as $\xi = 2M\ell$. In our model the $M = N - 1$ channels available for transport have the *same* group velocity $v = 2Va/\hbar$. This striking feature of the model allows to reach a one-dimensional diffusive dynamics when $N \to \infty$. For finite N it provides an optimal representation for one-dimensional excitations. We studied many system sizes and amounts of disorder, a typical evolution is shown in Fig. 1. The particular system for this figure has $N = 12$ and a perimeter of $100a$, $W = 3V$, $\ell \sim 6a$ and $\xi \sim 140a$. We see that after a ballistic time ℓ/v, the evolution follows a power law which indicates a diffusive behavior. Nevertheless, the exponent of this power law is somewhat different from the expected one-dimensional value 0.5. As in the examples mentioned above, this anomalous exponent could be due to a fractal effective dimension of the system. The fitting of the evolution to a power law with a free exponent resulted in an effective dimension of the system $d^* \sim 0.7$. In our model, a possible cause for a fractality in the eigenfunctions of the system is disorder. Strongly localized states in the band tails are confined around some random points. This means that they represent "holes" in the real space allowed to extended wave functions, thus making the effective dimension of the system smaller than the real one. For times longer than the ones shown in the figure, the autocorrelation function saturates, this is a finite size effect (the saturation value depends linearly on the system size). We also observed that a magnetic field does not change the exponent in the power law noticeably, but reduces the value of the saturation, meaning that there are fewer localized states. Another way to study how the eigenstates of energy ε are occupying some fraction of the volume of space is by means of the inverse participation number $p^{-1} = \sum_i |\varphi_i(\varepsilon)|^4$ [6]. For plane waves one obtains that $p = L^d$, i.e., it equals the volume of the system. For a localized state p is proportional to the volume in which the state has a non-vanishing amplitude. However, if the states are extended but fractal, in the thermodynamic limit it diverges as $p = L^{d^*}$, with d^* an effective dimension that may be different from the dimension d of the ordered system. We calculated the inverse participation number for each of the eigenstates of the system and through it the effective dimension ratio d^*/d of each of them. The results (shown in Fig. 2) are in very good agreement with the effective dimension calculated through the fitting of the autocorrelation function depicted in Fig. 1. Summarizing, we have introduced a numerical Hamiltonian model whose exact solution shows a regime with sub-diffusive behavior. Moreover, we presented hints of a fractal dimension of the extended eigenstates induced by the presence of disorder. By hindering particles from a fraction of the available real space, disorder induces a weak breaking of the ergodicity that anticipates the non-ergodicity associated with full localization.

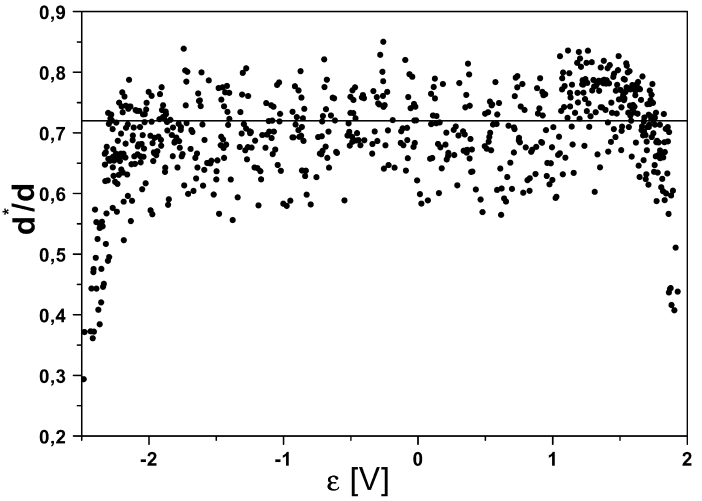

Fig. 2. Calculation of the effective dimension of every eigenstate of the system by means of the inverse participation number (dots) compared to the effective dimension obtained from the fitting of the dynamics of the system. Except for very localized states in the band edges, agreement is quite good.

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